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6. AUTHOR(S)
Morton E. Gurtin

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Carnegie-Mellon University
Pittsburgh, PA 15213

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13. ABSTRACT *(Maximum 200 words)*
The final report summarizes the research efforts on stability and thermal influences in nonlinear continuum mechanics and material science. Research on phase transitions included solid-solid phase transitions in deformable continua, evolution of interfacial curves and generalized Stefen problems. Studies were also made of general continuum mechanics.

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FINAL TECHNICAL REPORT SUMMARY

STABILITY AND THERMAL INFLUENCES IN NONLINEAR CONTINUUM MECHANICS AND MATERIAL SCIENCE

Grant DAAL03-91-G-0180

Principal Investigator: Morton E. Gurtin

Department of Mathematics, Carnegie Mellon

Tel: (412)268-2545 Fax: (412)268-6380 Email: mg0c@andrew.cmu.edu

1. Phase transitions

a. Solid-solid phase transitions in deformable continua

For a large class of two-phase problems discussed by materials scientists the material is presumed to be *rigid,* but there are situations in which deformation is important, examples being shock-induced transformations, twinning, and coarsening. [G8] develops a theory of solid-solid phase transitions in deformable continua, for a phase interface that is sharp and capable of supporting stress. A chief difficulty is the presence of *accretion,* the motion of the phase interface relative to the underlying material. The interplay between accretion and deformation requires a kinematics more complicated than that standard in continuum mechanics, and the mechanical description of accretion requires—over and above the standard forces that balance momentum—additional *configurational* forces with their own balance. The results of [G8] consist of free-boundary conditions relating jumps in bulk quantities to interfacial quantities such as surface stress and energy. The classical entropy relation of the theory of shocks is replaced by an *identity* that might have strong consequences in the theory of shock-induced phase transitions.

In the theory of [G8] the transition is *coherent;* that is, the reference lattices (homogeneous reference configurations) of the individual phases are coincident, and the deformation is continuous across the interface. In collaboration with Cermelli (U. Torino) [G11] (cf. [G14,G15]), a fairly complete kinematics is developed for *incoherent* phase transitions. Such transitions are more difficult to treat than their coherent counterparts. The interface, which appears as a single surface in the deformed configuration, is represented in its undeformed state by a separate surface in each phase. This leads to a rich but detailed kinematics, one in which defects such as vacancies, interstitials, and dislocations are generated by the moving interface. Associated with each two-phase motion are three basic kinematical quantities: an incoherency tensor that measures the stretching and twisting of one phase relative to the other; the production-rate of lattice points; and

the relative slip between phases. We show that these quantities completely characterize incoherency: an initially coherent motion is coherent for all time if and only if, at each time, the incoherency tensor is the identity, and the slip and lattice-point production vanish identically.

In [G15] (with Cermelli) a complete thermomechanics is developed for incoherent phase transitions in the presence of deformation and mass transport, with the phase interface structured by energy and surface stress. A new form of surface stress—not present when the interface is coherent—arises in response to the stretching and twisting of one phase relative to the other, thereby describing forces associated with the dislocation-content of the interface. The final results consist of a complete set of interface conditions for an evolving incoherent interface.

When a phase is quenched into a metastable state, the late stages of the phase transformation process are usually characterized by a dissolution of second-phase domains with large interfacial curvature at the expense of domains with low interfacial curvature. This process, known as coarsening (Ostwald ripening), occurs in a wide variety of two-phase materials. In spite of the wealth of experimental data showing that elastic stress has a profound influence on the morphological development of particles during ripening in solids, there is no continuum-mechanical framework that is dynamical and of sufficient generality to study two-phase phenomena in which deformation and stress accompany mass transport. Such a framework is the subject of joint research with Voorhees (Northwestern); [G3,G5], our first efforts, present a theory for linearly elastic bulk phases and surface energy, without surface elasticity.

Fried (Penn State) and I have been developing a theory of phase transitions characterized by an order parameter [G13] (cf. [G7]), one goal being a theory that yields dynamical problems that are computationally tractable. The chief ingredient of our approach is the characterization of phase through a list of order parameters. Order parameters can often be identified with microphysical concepts, but even when such identifications are difficult or even impossible, the introduction of order parameters can regularize the underlying theory in a manner that we believe to be at least conceptually well grounded. Within our theory, sharp phase-interfaces are replaced by *narrow transition zones* in which the strain and order parameter suffer large gradients. The addition of material to one phase at the expense of the other, here characterized by the order parameter, renders the theory conceptually different from the more standard theories of continuum mechanics. Motivated by the sharp-interface theory, microforces are introduced; these forces perform work over order-parameter changes and are consistent with their own force balance, which with the more standard momentum balances form the basic balance laws of the theory. By studying one-dimensional traveling waves and the asymptotics of a transition layer in three dimensions, connections between the theory based on an order parameter and the sharp interface theory are established. The additional balance for the microforces corresponds, asymptotically, to the configurational balance of the sharp interface theory as well as to an Euler-Lagrange equation derived variationally for the equilibrium theory, giving added credence to this additional balance.

The general theory allows for anisotropy and a full range of transition kinetics.

b. Evolution of interfacial curves

In planar two-phase heat conduction with interfacial energy and transition kinetics, when the thermal conductivities of the two phases are large, the underlying equations are formally approximated by a single equation

$$B(\theta)V = G(\theta)K - U \qquad (V = \text{normal velocity},\ K = \text{curvature}) \tag{1}$$

for the phase interface. Here $G(\theta)=f''(\theta)+f(\theta)$, $f(\theta)$ is the interfacial energy as a function of the angle θ to the interface normal, $B(\theta)>0$ is a kinetic modulus, and U is a constant difference in bulk energies. Equation (1) is *parabolic* for $G(\theta)>0$ and *backward-parabolic* for $G(\theta)<0$. [G1], written in collaboration with Angenent (Wisconsin), establishes the well-posedness of the corresponding initial-value problem and discusses the asymptotic behavior of its global solutions. For a realistic class of energies, $G(\theta)<0$ for some angle intervals; such backward-parabolic intervals are ruled out in [G1] by the introduction of corners (jumps in θ); in this case the capillary force

$$\mathbf{C}(\theta) = f(\theta)\mathbf{T}(\theta) + f'(\theta)\mathbf{N}(\theta) \quad \text{must be continuous across corners.} \tag{2}$$

Here $\mathbf{T}(\theta)$ and $\mathbf{N}(\theta)$ represent a unit normal and unit tangent to the interface.

The analysis of [G1] is inapplicable when the initial interface contains normal angles θ in the backward-parabolic range. [G2], written with DiCarlo and Podio-Guidugli (U. Rome), derives a physically consistent regularization of (1),

$$B(\theta)V = G(\theta)K - U - \varepsilon(2K_{ss} + K^3), \tag{3}$$

that may be used to study interfacial behavior in the backward-parabolic range. Here s denotes arc length and $\varepsilon>0$ is a small material parameter. The chief ingredient in the derivation of (3) is a constitutive dependence of interfacial energy on curvature, an idea that traces back to Gibbs and Herring. The equation (3) is very much like the Cahn-Hilliard equation, the angle-intervals on which $G(\theta)<0$ playing the role of spinodals.

Another method of removing the backward-parabolic behavior is to allow the interface to develop infinitesimal wrinkles over backward-parabolic intervals. This leads, at least formally, to a relaxed evolution equation of the form (1), in which $f(\theta)$ is replaced by its convexification (as a function on R^2) and $B(\theta)$ is modified also. For the relaxed equation, $G(\theta)=0$ over certain angle-intervals, with $G(\theta)$ generally not continuous at the endpoints of these intervals, while $B(\theta)$ remains continuous and strictly positive. Soner (Carnegie Mellon), Souganidis (Wisconsin), and I have developed a theory of (1) for moduli $G(\theta)$ of this type [G9]. Because of the lack of continuity

of G as well as the degeneracy of (1) when G=0, this equation is treated within the weak framework of viscosity solutions. Such weak solutions satisfy the force balance (2) and hence furnish a weak extension of the classical solutions developed in [G1]. [G9] establishes, for evolution from a given compact region: a theorem of existence and local uniqueness; a global comparison theorem for level-set solutions; and a theorem on the asymptotic behavior of solutions that grow without bound. Global comparison yields a justification of the relaxed equation by showing that if, given a smooth initial interface, we approximate each backward-parabolic section by an appropriate finitely wrinkled subcurve whose normal angles are "parabolic", then the resulting "classical solution" tends to the solution of the relaxed equation as the "amplitude" of the wrinkles tends to zero.

[G10] presents a comprehensive summary of work on evolving phase boundaries.

c. Generalized Stefan problems

The general two-phase Stefan problem with supercooling and superheating, but without capillarity, is difficult to formulate and solve, chiefly because of instabilities induced by supercooling and superheating. [G6] formulates this problem within a thermodynamical framework, the crucial ingredient being an appropriate entropy inequality and, in some cases, an entropy balance. This entropy balance and balance of energy yield distributional PDE's that provide a weak formulation of the two-phase problem, a formulation that differs from standard treatments in the use of an entropy balance to capture the classical Stefan condition, u=0 on the interface. Using this formulation it seems possible to discuss a wide range of physical phenomena, such as hypervelocity propagation of phase boundaries.

Matias (Carnegie Mellon) and I have developed a general Stefan problem in which the interfacial energy, as a function of orientation (normal), is restricted to a finite set, thereby yielding a fully-faceted interface [G12]. Bulk diffusion is included; the resulting free-boundary problem is nonstandard.

In [G16] (with Angenent, U. Wisconsin) generalized contact-angle conditions are developed for free surfaces such as phase interfaces; the resulting theory allows for crystal anisotropy as well as kinetics. To the our knowledge this is the first theory in which the contact condition has a dynamical contribution (in agreement with experiments)

2. General continuum mechanics

Ericksen and Toupin, in their theories of liquid crystals and oriented hyperelastic materials, introduce an additional equation expressing "balance of microforces". In [G4], written with Podio-Guidugli, this additional balance is derived as a consequence of invariance under changes in observer and a scaling that allows interaction between the macro- and micro-structural variables.

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